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The ionization equilibrium of iron in H II regions

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Abstract. We study the ionization equilibrium of Fe using photoionization models that incorporate improved values for the ionization and recombination cross-sections and the charge-exchange rates for the Fe ions. The previously available photoionization models predict concentrations of Fe^{3+} which are a factor of 3–8 higher than the values inferred from emission lines of [Fe III] and [Fe IV]. Our new models reduce these discrepancies to factors of 2–5. We discuss the possible reasons behind the remaining discrepancies and present an updated ionization correction factor for obtaining the Fe abundance from the Fe^{++} abundance.

1. Introduction

Iron is expected to be in two main ionization states in H II regions: Fe^{++} and Fe^{3+} (with the Fe^{+} ion having a non negligible concentration only for very low excitation nebulae). Therefore, the measurement of Fe III and Fe IV emission lines will allow us to determine the Fe abundance in these nebulae. [Fe III] lines, although weak, have already been observed in several H II regions and starburst galaxies (e.g. Izotov & Thuan 1999; Rodríguez 2002), but [Fe IV] lines are much weaker and difficult to observe. Therefore, the Fe abundance in H II regions is usually obtained from [Fe III] lines and an ionization correction factor (ICF), obtained from ionization models, to account for the contribution of Fe^{3+}. For example, the relation:

$$\frac{\mathrm{Fe}}{\mathrm{O}} = \mathrm{ICF}\,\frac{\mathrm{Fe}^{++}}{\mathrm{O}^{+}} = \frac{x(\mathrm{O}^{+})}{x(\mathrm{Fe}^{++})}\frac{\mathrm{Fe}^{++}}{\mathrm{O}^{+}}, \tag{1}$$

where $x(X^{n+})$ stands for the ionization fraction of the X^{n+} ion, is especially well suited for determining the Fe abundance from optical observations of H II regions. The ionization potentials of the O and Fe ions are similar (30.6 and 54.8 eV for Fe^{++} and Fe^{3+}, 35.3 and 54.9 eV for O^{+} and O^{++}). Furthermore, since both O^{+} and O^{++} can be measured from strong optical lines, one can get the O abundance $O/H = O^{+}/H^{+} + O^{++}/H^{+}$, and hence also Fe/H from Fe/O.

However, available measurements of some weak [Fe IV] lines (Rubin et al. 1997; Rodríguez 2003) imply Fe^{3+} abundances which are smaller than the values implied by relation (1) by factors 3–8. This discrepancy translates into an uncertainty of up to a factor of 6 in the Fe abundances derived for a wide range of objects, from the nearby Orion nebula to the low metallicity blue compact galaxy SBS 0335−052. Thus, resolving this problem has important implications for our understanding of both the evolution of dust in H II regions and the chemical history of low metallicity dwarf galaxies (see the contribution by Rodríguez & Esteban in this volume).

In order to check whether the discrepancy is due to errors in the ICFs predicted by models, we are studying the ionization equilibrium of Fe using photoionization models that incorporate recently improved values for all the atomic data relevant to the problem.

2. Results and discussion

We use the photoionization code NEBULA (Rubin et al. 1991a,b) with the following updates: new photoionization cross sections for Fe^{+}, Fe^{++}, O^{0} and O^{+} (Nahar & Pradhan 1994; Nahar 1996a; Kjeldsen et al. 2002; Verner et al. 1996), new recombination coefficients for Fe^{++}, Fe^{3+}, O^{+} and O^{++} (Nahar 1996b, 1997, 1999), all the charge-exchange reactions involving these ions (Kingdon & Ferland 1996; and the ORNL/UGA Charge Tranfer Database for Astrophysics — http://www-cfade.phy.ornl.gov/astro/ps/data); and the NLTE model stellar atmospheres of Pauldrach et al. (2001) with solar metallicity.

The ionization cross sections are not smoothly varying; they show several resonances at different energies. Since the positions of these resonances have uncertainties of a few percent, we smoothed (or used available smooth fits) both the ionization cross sections and the model atmospheres by convolving with Gaussians of widths 3% and 1.5% (in energy), respectively.

Figure 1 shows the ICFs obtained from different models with $T_{\rm eff} = 35000$–50000 K, total nucleon density $N = 100$–10000 cm^{-3}, and Orion metallicity Z, Z/10, and Z/30. The results of previous ionization models are also shown for comparison. The model results are compared with the results obtained by Rodríguez (2003) for several objects with available measurements of [Fe IV] lines. The new model results, although still higher than the measured values, are much closer to them. The remaining discrepancies could be due to: (1) the need for further improvements in the photoionization models, (2) errors in the atomic data (in particular the collision strengths) used to derive the Fe^{++} and Fe^{3+} abundances. The effect on the calculated values of $x(O^{+})/x(Fe^{++})$ of either decreasing the Fe^{++} abundance or increasing the Fe^{3+} abundance by a factor of 2 is also shown in Figure 1. This change would make the results for IC4846, 30 Doradus (its upper limit), and M42 compatible with the model results. The possibility of such a change is provided by the recent calculations of collision strengths for Fe^{++} by McLaughlin et al. (2002). However, they only calculate the collision strengths for transitions between terms. Hence, the new collision strengths cannot be used either to derive abundances or to check their reliability by comparing their predictions with the observed relative intensities of various [Fe III] lines.

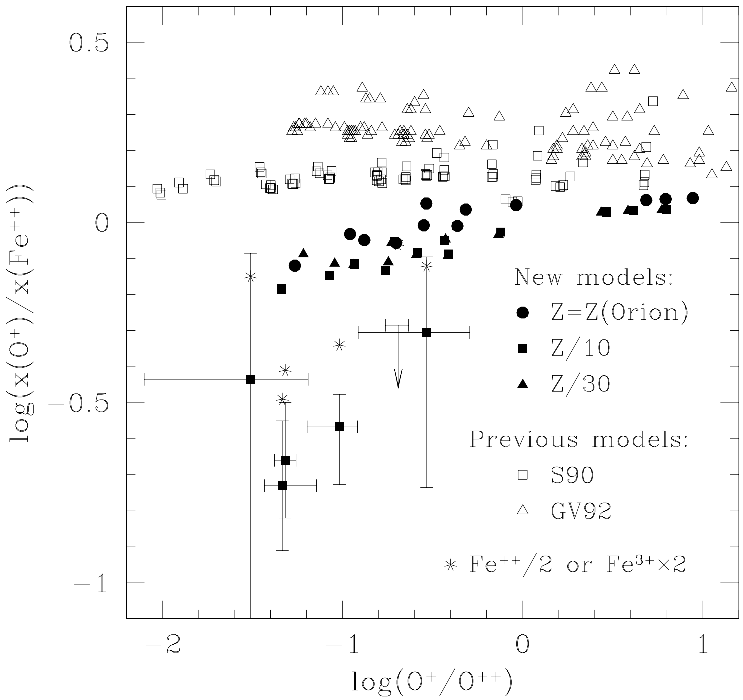

Figure 1. ICFs obtained from our new models compared with the previous model results of Stasińska (1990, S90) and Gruenwald & Viegas (1992, GV92). The squares with error bars show the results obtained in Rodríguez (2003) for objects with available measurements of [Fe IV] lines: from left to right, the planetary nebula IC4846, SMC N88A (one position in the object), the low metallicity blue compact galaxy SBS 0335−052, SMC N88A (a second position), 30 Doradus (an upper limit), and M42 (the Orion nebula). The asterisks show the effect on the calculated values of either decreasing the Fe^{++} abundance or increasing the Fe^{3+} abundance by a factor of 2.

Even if the factor of 2 decrease in the Fe^{++} abundance proved to be real, it would not explain the discrepancies shown by the objects with lower metallicities, SMC N88A and SBS 0335−052. However, the models with lower metallicity show slightly lower values for the ICF; thus further refinements (such as the use of low metallicity model atmospheres) might improve the fit. On the other hand, since different [Fe IV] lines were used to derive the Fe^{3+} abundance for the five objects, changes in the relevant collision strengths might explain all the discrepancies.

In any case, the Fe abundances implied by [Fe III] emission lines should be obtained through the relation implied by a fit through the new model results in Figure 1:

$$\frac{\mathrm{Fe}}{\mathrm{O}} = \left(\frac{\mathrm{O}^+}{\mathrm{O}^{++}}\right)^{0.09} \frac{\mathrm{Fe}^{++}}{\mathrm{O}^+}. \qquad (2)$$

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